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Soviet proposals

PROPOSALS FOR U.S. - SOVIET EXCHANGE PROGRAM
IN THE AREA OF CHEMICAL CATALYSIS

Proposal No.	Title
1	Fundamental research and development in the area of new applications of catalysis by metalorganic complexes in organic chemistry and petrochemistry ✓
2	Catalytic methods for the conversion of pollutants in exhaust gases and the possibility of applying catalysis to the purification of waste waters ✓
3	Mathematical methods and the use of computers in the study of catalysis ✓
4	The design of high ~~pressure~~ capacity reactors. ✓
5	Fundamental study of catalyst design for both deep and selective oxidation ✓
6	Application of catalysis to life support systems used in space exploration ✓

Some additional problems may be proposed after discussion with our American colleagues.

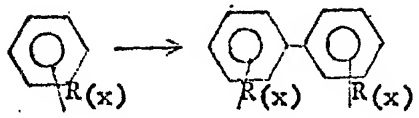
I. The scientific basis for and the search for new applications for catalysis by metal organic complexes in organic chemistry and petroleum chemistry

The development of catalytic systems capable of accelerating nucleophilic substitution reactions at a double bond (for oxidative coupling of aromatic hydrocarbons with each other and with olefins, the combination of olefins, etc.), polymerization, oxidation.

Both sides will select 5-10 relevant reactions, will divide them up amongst themselves, will then search for suitable catalytic systems and exchange results. When suitable systems or reactions are discovered both sides will negotiate a cooperative development program.

On the theoretical side, studies are proposed in the areas of the effect of ligands on the catalytic activity, the kinetics of the reaction, the mechanism of the elemental step, the effect of the structure of the starting materials on reactivity.

Examples of reactions:



$C_6H_6 + CH_3COOH \longrightarrow C_6H_5OOC - CH_3$

$2\ R\ CH{=}CH_2 \longrightarrow R{-}CH{=}CH{-}CH{=}CH{-}R$

II. Catalytic methods for the detoxification of exhaust gases and the possibility of using catalysis for the purification of waste waters

1. The scientific basis for the afterburning and decomposition of pollutants in the exhaust from vehicles and stationary engines. The development of new catalysis which could be more active (i.e., work at lower temperatures) and would be more available and less expensive.

The exchange of information and, possibly, the exchange of catalysts.

2. The investigation of catalytic methods useful for the removal of sulfur compounds, phenols, and other organic matter from waste water. This would include homogeneous as well as heterogenous methods.

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III. Mathematical methods and the use of computers in the study of catalysis

At present mathematical methods are widely used in all phases of catalytic investigations. The following directions are envisaged:

1. The use of mathematics in the planning of experimental programs in the area of catalysis and in the interpretation of the results.

2. The qualitative investigation of differential equations in ordinary and specific derivatives which describe catalytic processes (establish whether solutions exist, how many, their stability, etc.)

3. Mathematical methods for the optimization of catalytic processes (the principles of maximization, linear and non-linear programming, etc.)

4. The numerical methods for analysis of mathematical models of catalytic systems using computers.

5. Mathematical means for the interfacing of computers with experimental laboratory and pilot plant installations.

IV. The Construction of High Capacity Reactors

The increasing tempo of development in chemical industry requires the search for new ways and principles for the construction of high capacity reactors. The problems consist of several parts:

1. The scientific basis for the construction of reactors (modeling, optimization and fluid dynamics).

2. The problem of reliability in long term service.

3. The construction of reactors of high capacity on the basis of two and three phase fluidized beds.

4. The stabilization of unstable stationary conditions of operation.

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V. The scientific basis for the selection of catalysts for total and selective oxidation

General methods for selecting oxidation catalysts.

The development of catalysts for the preparation of different products (for example, epoxides, acrylonitrile, etc., by selective oxidation of olefins and paraffins.

The study of the mechanism of selective oxidation processes by kinetic and physical methods.

The study of the structure of oxidation catalysts.

VI. Application of catalysis to life support systems used in space exploration

In the U.S.S.R. the work is being carried out in the Institute of Medical-Biological problems (Ministry of Public Health of the U.S.S.R.), the Institute of Chemical Physics (Acad. of Science of the U.S.S.R.) and in other centers. There is a program for the exchange of information with American scientists working with NASA.

A cooperative study is proposed on the kinetics of condensation of formaldehyde into carbohydrates, information exchange on the kinetics of reactions over various catalysts, the search for new catalysts, the development of analytical methods for complex mixtures of carbohydrates and toxicological tests.

The theoretical consideration of various reaction schemes for the utilization of CO_2.

The questions of catalytic combustion of liquid and solid wastes will be considered in connection with the balance between formation and consumption of carbon dioxide.

The form of cooperation will involve the exchange of reports and of preprints of articles prior to their publications.